Approaching the Ground State of a Quantum Spin Glass using a Zero-Temperature Quantum Monte Carlo

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Here we discuss the annealing behavior of an infinite-range $\pm J$ Ising spin glass in presence of a transverse field using a zero-temperature quantum Monte Carlo. Within the simulation scheme, we demonstrate that quantum annealing not only helps finding the ground state of a classical spin glass, but can also help simulating the ground state of a quantum spin glass, in particularly, when the transverse field is low, much more efficiently.

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Quantum annealing (QA)[1-10] is a method of finding the ground state (minimum energy state) of a given classical Hamiltonian employing external quantum fluctuations and subsequent adiabatic reduction of them. In QA, one is given with a complex classical Hamiltonian $\mathcal{H}$ whose ground state is to be determined. In order to introduce the quantum fluctuations (necessary for the annealing) into the system, one adds a quantum kinetic term $\mathcal{H}'(t)$ to the classical Hamiltonian, such that $\mathcal{H}'(t)$ and $\mathcal{H}$ do not commute. Initially, one keeps $\mathcal{H}'(t=0) \gg \mathcal{H}$ so that the total Hamiltonian $\mathcal{H}_{tot}(t) = \mathcal{H}'(t) + \mathcal{H}$ is well approximated by the kinetic part only ($\mathcal{H}_{tot}(0) \approx \mathcal{H}'(0)$). The system is initially prepared to be in the ground state of $\mathcal{H}'(0)$ (one chooses $\mathcal{H}'(0)$ to have a easily realizable ground state). Now since $\mathcal{H}_{tot}(0) \approx \mathcal{H}'(0)$, the overlap $|\langle\psi(t)|\phi_1(t)\rangle|$ between the lowest eigen-value state (we will call it instantaneous ground state) $|\phi_1(t)\rangle$ of the total Hamiltonian $\mathcal{H}_{tot}(t)$ and the instantaneous state $|\psi(t)\rangle$ of the evolving system will be close to unity at $t = 0$ (since $|\psi(0)\rangle$ is taken to be the ground state of $\mathcal{H}'(0)$). If one subsequently reduces $\mathcal{H}'(t)$ slowly enough, then according to the adiabatic theorem of quantum mechanics, the overlap $|\langle\psi(t)|\phi_1(t)\rangle|$ will always stay close to its initial value (i.e., unity). Hence at the end of such an evolution, when $\mathcal{H}'(t)$ is reduced to zero at $t = \tau$, the system will be found in a state $|\psi(\tau)\rangle$ with $|\langle\psi(\tau)|\phi_1(\tau)\rangle| \approx 1$, where $|\phi_1(\tau)\rangle$ is the ground state of $\mathcal{H}_{tot}(\tau)$, which is nothing but the surviving classical part $\mathcal{H}$ of the Hamiltonian. Thus at the end of an adiabatic annealing the system is found in the ground state of the classical Hamiltonian with a high probability. Based on this principle, algorithms can be framed to anneal complex physical systems like spin glasses as well as the objective functions of hard combinatorial optimization problems (like the traveling salesman problem or TSP) mapped to glass like Hamiltonians, towards their ground (optimal) states.

Here we study the annealing behavior of an infinite-range $\pm J$ Ising spin glass in a transverse field, using a zero-temperature quantum Monte Carlo. The model and the basic QA scheme for it are introduced in Sec I. In Sec. II we discuss at length the zero-temperature quantum Monte Carlo method used here. We discuss the results of QA employed to reach the ground state of the classical spin glass in Sec. III. We demonstrate in Sec. IV, how QA can be utilized to simulate the ground state of a quantum spin glass. We conclude with a short summary.

I. MODEL

We consider an infinite range Ising spin system whose Hamiltonian is given by

$$\mathcal{H} = -\sum_{i,j(>i)}^{N} J_{ij}\sigma_i^z\sigma_j^z, \tag{1}$$

where σ_i^z is the $z-$component of Pauli spin, representing a classical Ising spin at site i and J_{ij}'s are random variables taking up values either $+1$ or -1 with equal probabilities. The above Hamiltonian describes a cluster of N Ising spins, each connected to all others through exchange interactions of equal strength ($J = 1$) but random signs. To make the energy extensive in system-size, one has to scales the energy with a factor of $N^{3/2}$, as done in the rest of the article. The system is heavily frustrated (i.e., no spin configuration can satisfy all the bonds), due to the presence of both ferromagnetic and antiferromagnetic bonds in random fashion. The high degree of connectivity (i.e., the infinite range of the interactions) adds to the complexity of the problem. For such a system, finding the ground state spin configuration for any arbitrary given realization of interactions (the set of J_{ij}'s), is

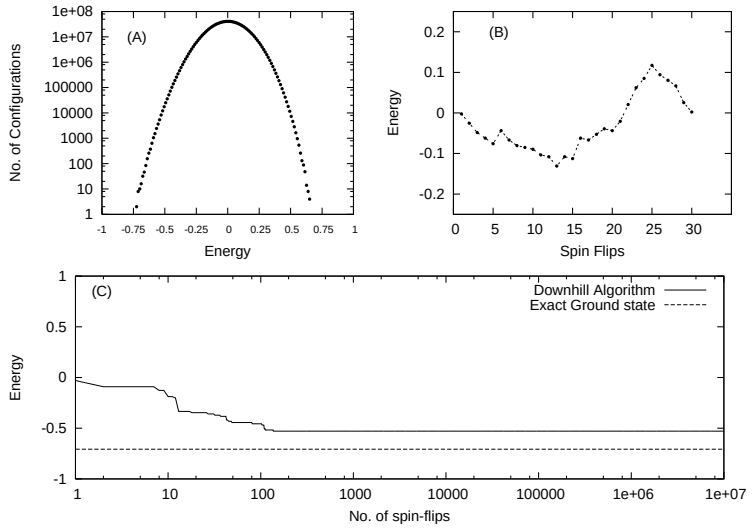

FIG. 1: Here the complexity of finding the ground state for a typical 30 spin sample of the $\pm J$ spin glass (Eq. 1) is illustrated. In (A) we plot the energy versus number of configurations for the sample. In (B) we plot the change in energy of the system as one flips the spins one-by-one, starting from a ferromagnetic (all up) state till the mirror symmetric one is reached. In Panel (C) we show how energy changes with time (spin flips) for a local downhill optimizer, who flips a spin randomly and accepts the move if it reduces the energy.

known to be an NP-hard problem[12]. In thermodynamic limit the system becomes a non-ergodic spin glass below some spin glass temperature T_G. To illustrate the complexity and the difficulty in finding the ground state we consider a typical sample with $N = 30$ (we studied many samples, and the features are qualitatively the same as we for this one) as shown in Fig. 1. The plot of the number of spin configurations against the energy (panel A of Fig. 1) of the system clearly shows that there is a huge entropy barrier between the ground state and the states which has higher energies. A levels with energy close to zero has a degeneracy of the order of 10^7, while the ground state degeneracy is of the order of unity. This problem could be easily overcome and ground state could be reached if the potential energy landscape (PEL) had have a more or less monotonic gradient towards the ground state, as observed in ferromagnetic samples (or may be one having few local non-monotonicity for samples with a few disorder and short-range interactions). But Here, as illustrated in panel (B), the PEL is quite random. In the Fig. 1(B), we plot the energy against spin flip, as we start from a completely ordered (all up) configuration and flip one-by-one all the 30 spins until the mirror-symmetric state (all down). In a ferromagnet, a similar plot would generate a convex curve (with the peak at the zero energy) symmetric about the energy axis, reaching the ground state at its both end. But here we find a completely random profile far above the real ground state energy. There is no helpful gradient to guide towards the ground state (if one incorporates moves with more than one spin-flips, then the profile becomes even more rugged). These two features, that is, the extremely low entropy of the ground state and the absence of a consistent gradient towards the ground state in the PEL makes it absolutely difficult for a random walker to find a ground state with the help of a naive local minimization algorithm, like the principle of going down hill, as shown in Fig. 1 panel (C). Here we show the energy of the system evolved using the random single spin-flip move, and allowing it to accept the move only if it minimizes the energy. We find even after 10^7 moves, it fails to reach the ground state. One can guess that after getting down in energy in first ~ 100 steps, it gets lost among the huge number of configuration with higher energies (which it does not accept) and cannot find a way to reach the sparsely occurring lower energy states.

The eigenstates of $\mathcal{H}$ (the basis states) are the direct-products of the eigenstates of σ_i^z's. Each basis state represents a distinct spin configuration of the system. To perform zero-temperature quantum annealing of this $\pm J$ Ising system, we add a transverse field term $\mathcal{H}' = \Omega(t)\sum_{i=1}^{N}\sigma_i^x$ where σ_i^x's are x-components of Pauli spins which introduces probability of tunneling between the basis states (classical configurations), and $\Omega(t)$ is the strength of the transverse field. The total Hamiltonian is thus given by

$$\mathcal{H}_{tot} = \mathcal{H} + \mathcal{H}'(t) = -\sum_{i,j(>i)}^{N} J_{ij}\sigma_i^z\sigma_j^z - \Omega(t)\sum_{i=1}^{N}\sigma_i^x. \quad (2)$$

We start with a high enough value of Ω initially (at $t = 0$) and sample the ground state of $\mathcal{H}_{tot}$ using a zero-temperature quantum Monte Carlo algorithm (discussed below). During sampling, we reduce the strength $\Omega(t)$ of the transverse field following a linear annealing schedule

$$\Omega(t) = \Omega_0(1 - t/\tau), \tag{3}$$

where t denotes evolution time. At the end of the simulation ($t = \tau$) we are left with the classical Hamiltonian $\mathcal{H}$ and if τ is large enough, the simulated system is finally found to be in one of its ground state configurations. For low values of τ, one generally ends up with a higher energy configuration.

II. THE ZERO TEMPERATURE QUANTUM MONTE CARLO METHOD

To simulate the ground state of $\mathcal{H}_{tot}$, we use a zero-temperature quantum Monte Carlo technique[11]. We describe the method to some details here, since it is not broadly known, and has been implemented so far only to simulate pure systems with short-ranged interactions. Here we generalize the implementation for an infinite-range system with disorders.

In this method one makes a linear transformation of the form

$$\mathcal{W} = C\mathcal{I} - \mathcal{H}_{tot}, \tag{4}$$

where C is a suitable real constant and $\mathcal{I}$ is the identity operator, such that the matrix representation of $\mathcal{W}$ in the eigen-basis of $\mathcal{H}$ is non-negative and irreducible (if such a transformation could not be done for an $\mathcal{H}_{tot}$, then this method would not be applicable for it). One can then consider $\mathcal{W}$ to be the transfer-matrix of a uniform chain (with Periodic Boundary Condition(PBC)) of classical plackets, where each placket is nothing but a classical cluster of N mutually interacting Ising spins represented by $\mathcal{H}$.

Now the key point is that one can simulate the chain of classical plackets using the elements of its transfer-matrix $\mathcal{W}$ and in this simulation the equilibrium average of any observable (say, energy) related to a single placket is approximately equal to the expectation value of the observable over the dominant eigenstate of $\mathcal{W}$. The dominant eigenstate of $\mathcal{W}$ in turn, is the ground state of $\mathcal{H}_{tot}$ (due to the form of the linear transformation between them). Thus we actually simulate the ground state properties of $\mathcal{H}_{tot}$ by simulating the chain. In the next section we establish the scheme in details.

A. Simulation of a chain of classical plackets using Transfer-matrix

In this subsection we demonstrate that the equilibrium averages for a single member of a uniform classical chain (with PBC) is approximately equal to the respective averages (expectation values) over the dominant eigenstate of the transfer-matrix of the chain. Let us consider a uniform chain of L identical classical spin clusters (or may be any localized discrete degrees of freedom in general) μ_i's, as shown in Fig. (2). Each of the μ_i's can be in, say, p different states. One may note here, that if each placket μ is a spin cluster embedded in dimension d, then the chain is actually a $d+1$-dimensional object. Since the chain is uniform, its Hamiltonian will be of the form

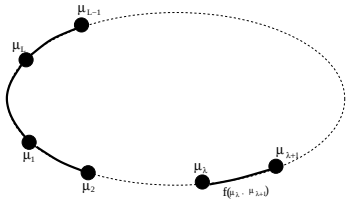

FIG. 2: The figure shows the uniform chain of plackets (with periodic boundary condition) used to simulate the ground state of $\mathcal{H}_{tot}$ (Eq. (2)). A placket (solid circle) in the chain is basically the cluster of N Ising spins with a given realization of J_{ij}'s, represented by $\mathcal{H}$ in Eq. (2). The interactions $f(\mu_\lambda, \mu_{\lambda+1})$ between any two nearest-neighbor-plackets are determined by the relation $\mathcal{W}_{\mu_\lambda\mu_{\lambda+1}} = e^{-\beta f(\mu_\lambda,\mu_{\lambda+1})}$, where $\mathcal{W}$ is obtained from $\mathcal{H}_{tot}$ by the linear transformation ((4)). If the dimension of each placket is d, then the dimension of the resulting chain is $d+1$.

$$\mathcal{H}_{d+1} = \sum_{\lambda=1}^{L} f(\mu_\lambda, \mu_{\lambda+1}),$$

where $f(\mu_\lambda, \mu_{\lambda+1})$ is a $p \times p$ matrix whose elements are the possible contributions to the Hamiltonian from a pair of neighboring spins, as each of them takes up p different values independently. The partition function of the chain is thus given by

$$\begin{aligned} Z &= \sum_{\mu_1=1}^{p} ... \sum_{\mu_L=1}^{p} \exp\left[-\beta \sum_{\lambda=1}^{L} f(\mu_\lambda, \mu_{\lambda+1})\right] \\ &= \sum_{\mu_1=1}^{p} ... \sum_{\mu_L=1}^{p} e^{-\beta f(\mu_1,\mu_2)} \times e^{-\beta f(\mu_2,\mu_3)} \times ... \times e^{-\beta f(\mu_L,\mu_1)} \\ &= \sum_{\mu_1=1}^{p} ... \sum_{\mu_L=1}^{p} \mathcal{W}_{\mu_1\mu_2} \times \mathcal{W}_{\mu_2\mu_3} \times ... \times \mathcal{W}_{\mu_L\mu_1}, \end{aligned}$$

where $\mathcal{W}_{\mu_\lambda\mu_{\lambda+1}} = e^{-\beta f(\mu_\lambda,\mu_{\lambda+1})}$, β being the temperature inverse. Again, since each of μ_λ and $\mu_{\lambda+1}$ can take up p independent values (i.e., can be in p independent states), $\mathcal{W}_{\mu_\lambda\mu_{\lambda+1}}$ defines a $p \times p$ matrix $\mathcal{W}$. Hence summing over all the indices from μ_2 to μ_L and recalling the rule of matrix multiplication one gets

$$Z = \sum_{\mu_1=1}^{p} (\mathcal{W}^L)_{\mu_1\mu_1} = Trace(\mathcal{W}^L).$$

The matrix $\mathcal{W}$ is a transfer-matrix for the chain. If the matrix $\mathcal{W}$ is symmetric then (it is not the necessary but

the sufficient condition) one can write

$$Z = \sum_{r=1}^{p} (\theta_r)^L,$$

where θ_r are the eigenvalues of $\mathcal{W}$ ordered by the index r, so that $|\theta_i| \geq |\theta_j|$ if $i < j$. Here a few points are to be noted. Since all the elements of $\mathcal{W}$ are strictly positive at any finite β, the matrix $\mathcal{W}$ is both non-negative and primitive (i.e., there exists some finite n, such that $\mathcal{W}^n$ is strictly positive). Then according to Perron-Frobenius theorem (see[13]) the dominant eigenvalue θ_1 is strictly positive and non-degenerate. Thus

$$\begin{aligned} Z &= (\theta_1)^L + \sum_{r=2}^{p} \left(\frac{\theta_r}{\theta_1}\right)^L \\ &\approx (\theta_1)^L \end{aligned}$$

Here, the leading order error is $(\theta_2/\theta_1)^L$ and since θ_1 is non-degenerate,

$$\lim_{L\to\infty} \left(\frac{\theta_i}{\theta_1}\right)^L = 0 \tag{5}$$

for any $i \neq 1$.

Now, to see how one can simulate the chain using $\mathcal{W}$, one has to note that the probability that the chain be in a given state A , in which $\mu_1 = \mu_1(A), \mu_2 = \mu_2(A)...$ etc, is

$$\begin{aligned} P(A) &= \left(e^{-\beta f[\mu_1(A),\mu_2(A)]} \times ... \times e^{-\beta f[\mu_L(A),\mu_1(A)]}\right)/Z \\ &= \left(\mathcal{W}_{\mu_1(A)\mu_2(A)} \times ... \times \mathcal{W}_{\mu_L(A)\mu_1(A)}\right)/Z \end{aligned} \tag{6}$$

Thus using the conditions of detailed balance, one obtains transition probability from a state A to another state B given by

$$P(A \to B) = \frac{\mathcal{W}_{\mu_1(B)\mu_2(B)} \times ... \times \mathcal{W}_{\mu_L(B)\mu_1(B)}}{\mathcal{W}_{\mu_1(A)\mu_2(A)} \times ... \times \mathcal{W}_{\mu_L(A)\mu_1(A)}}. \tag{7}$$

Thus if $\mathcal{W}$ is given, we can simulate the equilibrium properties (thermal average) of any physical quantity related to a placket μ in the chain. To obtain that, we require to know the probabilities for the placket μ to be in its different possible states when the chain is in equilibrium. Let $P(\mu = k)$ denotes the probability that the placket is found in its k-th state when the chain is at thermal equilibrium (at a given β). If the k-th state is represented by a column vector $|k\rangle$, then these column vectors satisfy the matrix relation

$$\langle i|\mathcal{W}|j\rangle = \mathcal{W}_{ij},$$

where $\langle i|$ is the transpose of $|i\rangle$ and the sequence of matrices implies the proper multiplications between them.

On the other hand, if $|E_1\rangle$ be the dominant (normalized) eigenvector of $\mathcal{W}$ corresponding to the dominant eigenvalue θ_1, and if $\mathcal{W}$ is hermitian then one can expand $|E_1\rangle$ linearly in terms of the basis vectors as

$$|E_1\rangle = \sum_{k=1}^{p} \gamma_1^k |k\rangle, \tag{8}$$

where γ_k^1 is the amplitude of the basis state $|k\rangle$ in $|E_1\rangle$. Thus in the sampling of $|E_1\rangle$ using the basis states $|k\rangle$'s, the probability of occurrence of the state $|k\rangle$ will be $|\gamma_k^1|^2$. Now, one can show that

$$P(\mu = k) = |\gamma_k^1|^2 + \mathcal{O}\left[(\theta_2/\theta_1)^L\right]. \tag{9}$$

The above equation says that one can sample the dominant eigenstate $|E_1\rangle$ of the matrix $\mathcal{W}$ just by sampling its basis states (classical configurations of a placket in the chain) according to the probability of their occurrence in the simulation of the placket at equilibrium in the chain (using the elements of $\mathcal{W}$ itself, as prescribed in (7)).

To prove equation (9), we take any placket in the chain and call it μ_1. Probability that μ_1 is found in the state $|k\rangle$ is

$$\begin{aligned} P(\mu_1 = k) &= \frac{1}{Z}\left[\sum_{\mu_2}\sum_{\mu_3}...\sum_{\mu_L} \mathcal{W}_{\mu_1\mu_2}\mathcal{W}_{\mu_2\mu_3}...\mathcal{W}_{\mu_L\mu_1}\right]_{\mu_1=k} \\ &= \frac{1}{Z}\left(\mathcal{W}\right)^L_{kk} = \frac{\langle k|(\mathcal{W})^L|k\rangle}{trace\{(\mathcal{W})^L\}} \end{aligned} \tag{10}$$

Above, we have summed up the probabilities of all the configurations of the chain, in which $\mu_1 = k$. Now let $|\theta_i\rangle$ $(i = 1, 2, ...p)$ denote the normalized eigenvector of $\mathcal{W}$ corresponding to the eigenvalue θ_i. Then one may have a linear transformation between $|\theta_i\rangle$'s and $|k\rangle$ of the form

$$|\theta_i\rangle = \sum_k \gamma_k^i |\mu_k\rangle$$

and the reverse transformation

$$|k\rangle = \sum_i (\gamma^\dagger)_i^k |\theta_i\rangle = \sum_i \gamma_k^{i*} |\theta_i\rangle,$$

γ being an unitary matrix. Hence

$$\begin{aligned} \mathcal{W}^L|k\rangle &= \sum_i \gamma_k^{i*}\theta_i^L|\theta_i\rangle \\ \Rightarrow \langle k|\mathcal{W}^L|k\rangle &= \sum_i |\gamma_k^i|^2\theta_i^L, \end{aligned}$$

using ortho-normality of $|\theta_i\rangle$'s. Thus, from equation (II A) we get

$$\begin{aligned} P(\mu_1 = k) & \\ &= \frac{\langle k|\mathcal{W}^L|k\rangle}{trace\{\mathcal{W}^L\}} \\ &= \frac{\sum_i |\gamma_k^i|^2\theta_i^L}{\sum_i \theta_i^L} \\ &= \frac{\sum_i |\gamma_k^i|^2(\theta_i/\theta_1)^L}{1 + \sum_{i\neq 1}(\theta_i/\theta_1)^L} \\ &\approx |\gamma_k^1|^2 + \mathcal{O}[(\theta_2/\theta_1)^L], \end{aligned}$$

which proves equation (9).

Thus one can in fact simulate the dominant eigenstate of any given suitable (hermitian, non-negative and primitive) $N \times N$ matrix up to a good approximation using the above results. One has to define a uniform chain (with PBC) of classical plackets, each having N possible configurations. The i-th state of a placket corresponds to the i-th vector of the basis in which the given matrix is represented. One then views the given matrix as the transfer-matrix for a placket in the chain, and simulate the chain using its elements (as prescribed in (7)). At equilibrium, the probability of getting a placket in its i-th state is equal to the modulus square of the weight of the i-th basis vector in the representation of the dominant eigenstate of the given matrix (up to an error of the form discussed above).

B. Implementation of the Monte Carlo

We now illustrate the implementation of the above Monte Carlo scheme by employing it to simulate the ground state of $\mathcal{H}_{tot}$ given in Eq. (2). Here basis vectors $|k\rangle$'s are the eigenvectors of $\mathcal{H}$, and a classical placket is the cluster of N Ising spins with exchange interaction described by $\mathcal{H}$. Now we make a linear transformation of the form given in Eq. (4), with $C = N(N-1)/2$. The resulting $\mathcal{W}$ matrix is clearly non-negative (since none of its diagonal element are all smaller than $N(N-1)/2$ and off-diagonal elements are either 0 or $\Omega(t)$, which we always take to be positive.). Since $\mathcal{H}_{tot}$ connects a basis state to all other basis states that can be obtained by a single spin flip from it, there is no closed subspace for $\mathcal{H}_{tot}$. Thus $\mathcal{W}$ is also irreducible. It can be shown that for a non-negative irreducible matrix, all the results of Perron-Frobenius theorem we have used here, holds good[13]. Besides, $\mathcal{W}$ is of course hermitian. Hence we can take $\mathcal{W}$ as a transfer-matrix for the chain. It corresponds to some interaction $f(\mu_\lambda, \mu_{\lambda+1})$ between two neighboring (μ_λ and $\mu_{\lambda+1}$) and some inverse temperature β (not explicitly important here), given by

$$\mathcal{W}(\mu_\lambda, \mu_{\lambda+1}) = e^{-\beta f(\mu_\lambda, \mu_{\lambda+1})}.$$

To simulate the ground state of $\mathcal{H}_{tot}$ at a given Ω for a particular realization of J_{ij}'s, we construct a uniform chain of L plackets with PBC. Each placket is a cluster of N classical Ising spins (described by cooperative term of $\mathcal{H}_{tot}$) connected through the given particular realization of J_{ij}'s (see (2)). We start with an arbitrary spin configuration (same for all plackets) and a given value of Ω. In one Monte Carlo step we randomly visit L plackets. At each such visit we make an allowed move (a move whose probability is not trivially zero), such that the chain goes from a state A, say, to a new state, say B. The probability of acceptance of the move is nothing but the transition probability $P(A \to B)$ calculated following (7) (using the elements of $\mathcal{W}$). While sampling, one can easily avoid moves whose probabilities are trivially zero (due to the sparsity of the matrix $\mathcal{W}$) by constructing a more restricted Markov process to do the sampling[11].

For doing quantum annealing of the same system, we start with a high enough value of Ω and reduce it very slowly with time t (Monte Carlo step) following a linear schedule. During visiting different plackets in a given Monte Carlo step, Ω is however held fixed. The linear schedule is specified by $\Omega(t=0) = \Omega_{in}$ and The total number of Monte Carlo steps executed; Ω_{in} is linearly reduced to zero with t within 95% of the total Monte Carlo steps, we thus have $\Omega(t) = \Omega_{in}(1 - t/\tau)$, where τ is the annealing time.

III. RESULTS AND DISCUSSIONS

We have studied the relaxation behavior of several random J_{ij} samples with $N = 30$ for linear annealing schedule (we start with an initial transverse field Ω_{in} and reduce it linearly with Monte Carlo step, so that it becomes zero before last few, 5%, steps. We observe that for an annealing of $\sim 10^7$ Monte Carlo steps, the system reaches the true ground state (determined by an extensive search method) in almost every case, for a suitably large initial transverse field Ω_{in}. We calculate the average exchange energy of the chain (over L plackets) in each Monte Carlo step, and average that over a few $\sim$ 500 Monte Carlo steps. The exchange energy (as given by $\mathcal{H}$ of Eq. (2) is not linear in N and we have to scale it by a factor $N^{3/2}$ to obtain the intensive energy density. In thermodynamic limit, this intensive energy density approaches the value -0.7633[15] (our finite size results shows some fluctuations about that). In Fig. (3) the relaxation behavior of three typical random realizations (R1, R2 and R3) during their annealing are shown. We found that for doing annealing of a given sample within a given number of steps, there is a suitable range of Ω_{in}. If Ω_{in} falls below the range, then the transition probabilities are too low to be able to anneal the system within the given time. On the other hand, if Ω_{in} is above the range, then the rate of change of $\Omega(t)$ is not slow enough to ensure the convergence to the ground state finally (i.e., the evolution in no more adiabatic). In Fig. (3), the values of respective Ω_{in}'s belong to the lower end of the respective ranges. The ranges are generally wide enough, and one can find a Ω_{in} within the range, just by a few trials.

The relaxation behavior is found to be typically "linear" in the sense that the long-time averages decrease linearly with time (see lower part of Fig. (4)). The relaxation observed in shorter time scale of course shows fluctuations around that linear behavior (shown in the upper part of Fig. (4)). This linear nature of relaxation is typically seen independent of the details of the particular realizations.

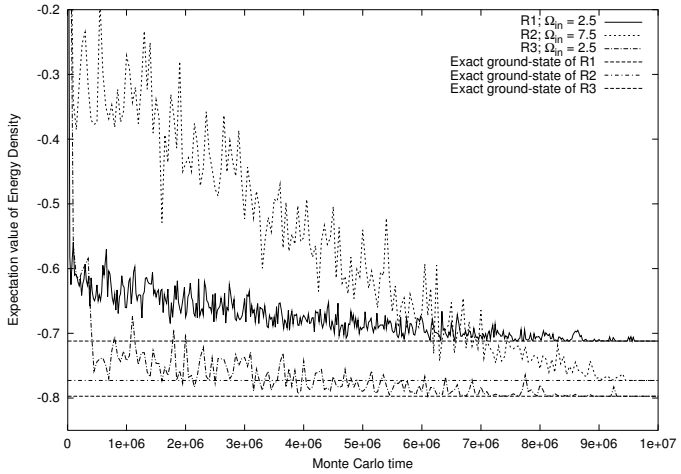

FIG. 3: In the figure, annealing behavior of three different randomly generated realizations (R1, R2 and R3) of J_{ij}'s are shown for $N = 30$. In Each case the system goes to the exact ground state (shown by respective horizontal lines) at the end of the annealing. In each case the annealing time is 10^7 Monte Carlo steps, number of plackets in the chain is $L = 600$, and each Monte Carlo step consists of visiting L plackets randomly and making a random spin-flip trial there. In each case, the transverse field has been reduced to zero from its initial value $\Omega_{in} = 5$ following a linear schedule, within the Monte Carlo steps.

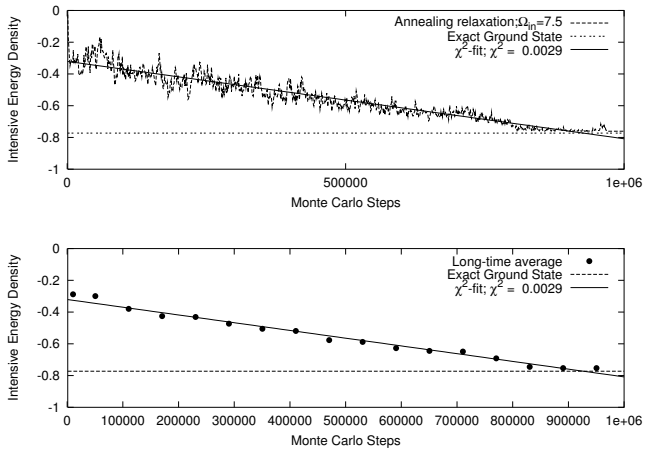

FIG. 4: In this figure the annealing relaxation ($N = 30$, $L = 600$ and $\Omega_{in} = 7.5$) for a particular realization is shown. Here the annealing time $\tau = 10^6$ Monte Carlo steps. The upper frame shows the relaxation of intensive energy density with time, when averaged over small (~ 500) Monte Carlo steps. The lower frame shows the same relaxation, when the averaging is done over a much larger number of ($\sim 10^4$) Monte Carlo steps. A linear χ^2-fit for the longer time average is shown in the lower part of the figure.

IV. BETTER SIMULATION OF LOW KINETIC-ENERGY QUANTUM STATES USING QUANTUM ANNEALING

In a glassy system, where the potential energy landscape has valleys separated by huge energy barriers, simulating the ground states (and possibly other low-lying states) for low kinetic energy (like the ground state for a low value of the transverse of a transverse Ising spin glass) using a zero-temperature quantum Monte Carlo may be very difficult and time consuming. This is because, for small kinetic term, the acceptance probability may become very small for higher potential energy states energy states, and the system may take a very long time to get out of a local potential energy minimum in order to visit other equally relevant lower-potential-energy valleys. Thus if one gets stuck is a local minimum far above the ground state, at an early, stage of the simulation, then it would not be able to reach the low lying valleys, whose contributions to the ground state are much more significant. This can be remedied to some extent by annealing the sample quantum mechanically starting with

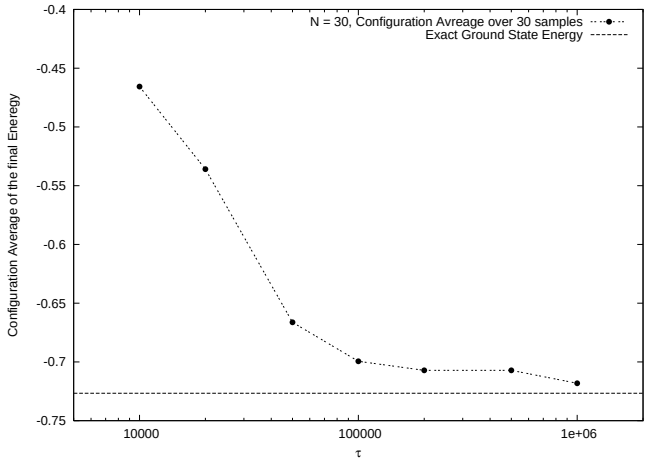

FIG. 5: Here the variation of the final energy with the annealing time τ is shown for the sample size $N = 30$. Each data point is averaged over the same set of 30 disorder configurations. The transverse field Ω is reduced linearly from $\Omega_{in} = 1.5$ and the replica number is taken to be $L = 600$. The horizontal line denotes the exact ground state (averaged over the same set of configurations) obtained by an exhaustive search algorithm.

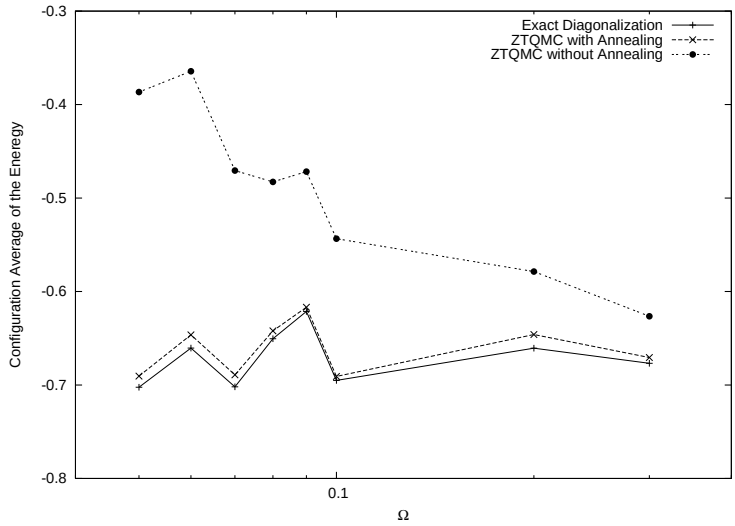

FIG. 6: In this figure a comparison between the results of simulation (with and without pre-annealing) of the ground state of the Hamiltonian (2) for different static values of Ω and the corresponding exact results obtained by numerical exact diagonalization for the same set of samples. Each data-point represents an average over the same set of 40 randomly generated samples of size $N = 20$. The total number of Monte Carlo steps is 10^5 for each Monte Carlo simulation (including the annealing period for the annealed simulations). In the figure, he results of simulations with annealing are seen to be much closer to the exact diagonalization results than those with out annealing. for lower values of Ω.

a high value of the kinetic energy, and then reducing it slowly up to the low value at which the simulation is desired.

For the Hamiltonian given by Eq. (2), simulation of the ground state for a small fixed value of the transverse field Ω (using the zero-temperature transfer-matrix Monte Carlo algorithm described here) is found to be much closer to the exact result (obtained using exact diagonalization[14]) when the simulation is done following an annealing (reducing Ω from a high value to the low value at which the simulation is desired) than that done directly keeping the value of Ω fixed to the low value from the onset. We compare the results of both kinds of simulations (with and without annealing), for several random samples of the spin glass for $N = 20$ with the respective exact diagonalization results for them (see Fig. 6).

We conclude summarizing few points regarding the performance of the algorithm described here. The algorithm discussed here is quite general (applicable to any disordered spin system in any dimension) and may be used for simulating small system-sizes quite satisfactorily. However, the moves are very restricted, since each

spin flip in a placket requires the two nearest-neighboring plackets to be in the same configuration with it. For large system sizes, this is too restrictive a condition to move freely enough through the configuration space to procure a satisfactory sampling rate. In addition, since the acceptance probability for higher potential energy configurations (like most other zero-temperature quantum Monte Carlo algorithms) depends on the magnitude of the kinetic term, it is hard to simulate the ground state for low values of the kinetic term. We have shown how quantum annealing can be utilized in overcoming this difficulty (at least partially). This remedy is is expected to work also for other zero-temperature quantum Monte Carlo methods in principle.

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